PDF Study of RuOH Hydroxides

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Introduction: Direct methanol fuel cells (DMFCs) are promising "green" power sources for electric vehicles. In the last decade, the efficiency of DMFC systems has been improved significantly. In the opinion of the majority of the fuel cell community the DMFC catalysts are most likely Pt-Ru bimetallic alloys. One of the major remaining problems is the relatively poor activity of the Pt-Ru catalysts used at the anode to oxidize methanol and irreproducibility in the catalyst performance. In order to improve the catalyst performance, it is important to understand the microscopic origin of the catalyst activity.

Methods and Materials: We have used monochromatic X-rays of 22 keV energy and solid-state Ge detector. Data were corrected for background, absorption and multiple scattering. Pair distribution function was obtained by means of Fourier transformation of the normalized structure factors. We examined several Ru hydroxides with different content of water.

Results: **Figure 1** shows the PDF of RuO_xH_y annealed at various temperatures. In these samples the ratio of RuO_2:H_2O, 1:x, changes from 1:0.84 for 100°C annealing to 1:0.02 for 400°C annealing. As water is removed from the system local atomic order extends to longer distances. It should be noted, however, that the peak positions up to 10 Å hardly change, and only the peak heights change with removal of water. The first peak at 1.96 Å corresponds to the Ru-O bond distance, and the next three major peaks (3.03, 3.56, 5.56 Å) are due to Ru-Ru distances in the rutile structure of RuO_2. Smaller peaks not present in the PDF of RuO_2, such as the one at 2.4 Å, must originate from the Ru-O distances involving water

Conclusions: The PDF peak values plotted against the water content in the sample indicate a clear change in the slope around x = 0.4. This composition approximately corresponds to the best composition for electron/proton mixed conduction, indicating that the structure is qualitatively different above and below this threshold.

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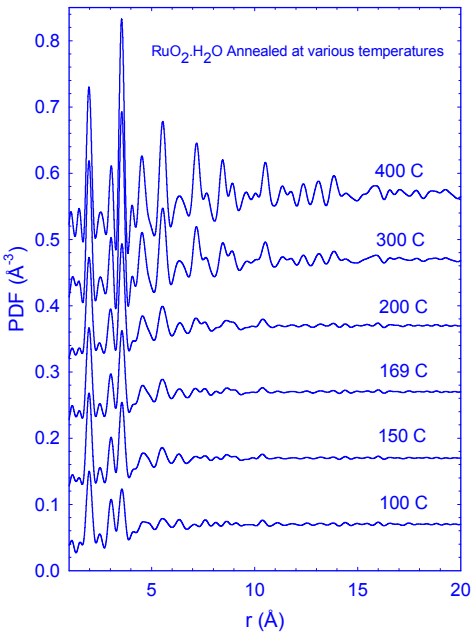

Figure 1. PDF of $RuO_2 \bullet (H_2O)_x$ annealed at various temperatures